New approach to (quasi)-exactly solvable Schrödinger equations with a position-dependent effective mass

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Abstract

By using the point canonical transformation approach in a manner distinct from previous ones, we generate some new exactly solvable or quasi-exactly solvable potentials for the one-dimensional Schrödinger equation with a position-dependent effective mass. In the latter case, SUSYQM techniques provide us with some additional new potentials.

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1 Introduction

In recent years, quantum mechanical systems with a position-dependent effective mass (PDEM) have attracted a lot of attention due to their relevance in describing the physics of many microstructures of current interest, such as compositionally graded crystals [1], quantum dots [2], ^{3}He clusters [3], quantum liquids [4], metal clusters [5], etc.

As in the constant-mass case, exact solutions play an important role because they may provide both a conceptual understanding of some physical phenomena and a testing ground for some approximation schemes. Many recent developments have been devoted to constructing exactly solvable (ES), quasi-exactly solvable (QES) or conditionally-exactly solvable potentials for the PDEM Schrödinger equation [6]–[17] by using point canonical transformations (PCT), Lie algebraic techniques or supersymmetric quantum mechanical (SUSYQM) methods.

In this Letter, we will show that new ES or QES potentials in a PDEM background may be generated by using the PCT approach in a manner distinct from previous ones. We will then combine such results with SUSYQM methods to produce some additional QES potentials.

2 PCT approach in a PDEM context

As is well known (see, e.g., [14]), the general Hermitian PDEM Hamiltonian, initially proposed by von Roos [18] in terms of three ambiguity parameters α, β, γ such that $\alpha + \beta + \gamma = -1$, gives rise to the (time-independent) Schrödinger equation

$$H\psi(x) \equiv \left[-\frac{d}{dx} \frac{1}{M(x)} \frac{d}{dx} + V_{\text{eff}}(x) \right] \psi(x) = E\psi(x), \tag{1}$$

where the effective potential

$$V_{\text{eff}}(x) = V(x) + \frac{1}{2}(\beta + 1)\frac{M''}{M^2} - [\alpha(\alpha + \beta + 1) + \beta + 1]\frac{M'^2}{M^3} \tag{2}$$

depends on some mass terms. Here a prime denotes derivative with respect to x, $M(x)$ is the dimensionless form of the mass function $m(x) = m_0 M(x)$ and we have set $\hbar = 2m_0 = 1$.

Let us look for solutions of Eq. (1) of the form

$$\psi(x) = f(x) F(g(x)), \tag{3}$$

where $f(x)$, $g(x)$ are two so far undetermined functions and $F(g)$ satisfies a second-order differential equation

$$\ddot{F} + Q(g)\dot{F} + R(g)F = 0, \tag{4}$$

where a dot denotes derivative with respect to g. Since in this Letter we shall be interested in bound-state wavefunctions, we shall actually restrict ourselves to polynomial solutions of Eq. (4).

On inserting Eq. (3) in Eq. (1) and comparing the result with Eq. (4), we arrive at two expressions for $Q(g(x))$ and $R(g(x))$ in terms of $E - V_{\rm eff}(x)$ and of $M(x)$, $f(x)$, $g(x)$ and their derivatives. The former allows us to calculate $f(x)$, which is given by

$$f(x) \propto \left(\frac{M}{g'}\right)^{1/2} \exp\left(\frac{1}{2}\int^{g(x)} Q(u)\, du\right), \tag{5}$$

while the latter leads to the equation

$$E - V_{\rm eff}(x) = \frac{g'''}{2Mg'} - \frac{3}{4M}\left(\frac{g''}{g'}\right)^2 + \frac{g'^2}{M}\left(R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2\right) - \frac{M''}{2M^2} + \frac{3M'^2}{4M^3}. \tag{6}$$

It is clear that we need to find some functions $M(x)$, $g(x)$ ensuring the presence of a constant term on the right-hand side of Eq. (6) to compensate E on its left-hand side and giving rise to an effective potential $V_{\rm eff}(x)$ with well-behaved wavefunctions.

In the constant-mass case, i.e., for $M(x) = 1$, this procedure has been thoroughly investigated [19, 20]. A similar study in the PDEM context looks more involved for two reasons: (i) there are now two unknown functions instead of only one and (ii) the usual square-integrability condition for bound-state wavefunctions has to be completed by the additional restriction $|\psi(x)|^2/\sqrt{M(x)} \to 0$ at the end points of the definition interval of $V(x)$ to ensure the Hermiticity of H in the Hilbert space spanned by its eigenfunctions [17].

In most applications of PCT that have been carried out so far in the PDEM context, the choice $M = \lambda g'^2$ or $g(x) = (1/\lambda)\int^x \sqrt{M(u)}\, du + \nu$ (where λ, ν are some constants) has been made (see, e.g., [12, 13, 14]). In the next two sections, we will explore the new possibilities offered by two other options, namely $M = \lambda g'$ and $M = \lambda/g'$ or, equivalently, $g(x) = (1/\lambda)\int^x M(u)\, du + \nu$ and $g(x) = (1/\lambda)\int^x [M(u)]^{-1}\, du + \nu$.

3 Generation of ES potentials in the $M = \lambda g'$ case

Substituting $M = \lambda g'$ into Eq. (6) leads to

$$E - V_{\rm eff}(x) = \frac{1}{\lambda} g' \left(R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2 \right). \tag{7}$$

Some simple and interesting results can be derived from this relation by assuming that $F(g)$ is either a Jacobi or a generalized Laguerre polynomial [21].

For $F_n(g) \propto P_n^{(a,b)}(g)$, $n = 0, 1, 2, \ldots$, $a, b > -1$, we obtain

$$\begin{aligned} R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2 &= \frac{n(n+a+b+1)}{1-g^2} + \frac{1}{(1-g^2)^2}\left[\frac{1}{2}(a+b+2) - \frac{1}{4}(b-a)^2\right] \\ &\quad + \frac{g}{(1-g^2)^2}\frac{1}{2}(b-a)(b+a) - \frac{g^2}{(1-g^2)^2}\frac{1}{4}(a+b)(a+b+2). \end{aligned} \tag{8}$$

A constant term can therefore be generated on the right-hand side of Eq. (7) by assuming $g'/[\lambda(1-g^2)] = C$, where C must be restricted to positive values in order to get increasing energy eigenvalues for successive n values. The solution of this first-order differential equation for $g(x)$ leading to a positive mass function reads $g(x) = \tanh qx$, where $q = \lambda C > 0$. Without loss of generality, we may set $C = q^2$ so that $\lambda = 1/q$. Hence we get

$$g(x) = \tanh qx, \qquad M(x) = \operatorname{sech}^2 qx, \qquad -\infty < x < +\infty. \tag{9}$$

Equations (5), (7), (8) and (9) then yield

$$E_n = q^2\left(n + \frac{a+b}{2}\right)\left(n + \frac{a+b+2}{2}\right) + V_0, \tag{10}$$

$$\begin{aligned} V_{\rm eff}(x) &= q^2\left\{\left[\frac{1}{2}(a^2+b^2) - 1\right]\cosh^2 qx + \frac{1}{2}(a-b)(a+b)\sinh qx \cosh qx\right\} + V_0 \\ &= \frac{1}{4}q^2\left[(a^2-1)e^{2qx} + (b^2-1)e^{-2qx} + a^2 + b^2 - 2\right] + V_0, \end{aligned} \tag{11}$$

$$\psi_n(x) \propto (1 - \tanh qx)^{(a+1)/2}(1 + \tanh qx)^{(b+1)/2} P_n^{(a,b)}(\tanh qx), \tag{12}$$

where $n = 0, 1, 2, \ldots$, V_0 denotes some constant and we have to assume $a, b > -1/2$ in order to satisfy the conditions on bound-state wavefunctions in a PDEM context (observe that the square-integrability condition alone does not impose any restriction on a, b!).

By proceeding similarly for $F_n(g) \propto L_n^{(a)}(g)$, $n = 0, 1, 2, \ldots$, $a > -1$, from the relation [21]

$$R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2 = \frac{2n+a+1}{2g} - \frac{(a+1)(a-1)}{4g^2} - \frac{1}{4} \tag{13}$$

and the condition $g'/(\lambda g) = C > 0$, we obtain the results

$$g(x) = e^{-qx}, \qquad M(x) = e^{-qx}, \qquad -\infty < x < +\infty, \tag{14}$$

where we have set $C = q^2$ (hence $\lambda = -1/q$) and where without loss of generality we may assume $q > 0$. Furthermore

$$E_n = q^2\left(n + \frac{a+1}{2}\right) + V_0, \tag{15}$$

$$V_{\rm eff}(x) = \frac{1}{4}q^2\left[(a^2-1)e^{qx} + e^{-qx}\right] + V_0, \tag{16}$$

$$\psi_n(x) \propto \exp\left\{-\frac{1}{2}\left[(a+1)qx + e^{-qx}\right]\right\} L_n^{(a)}\left(e^{-qx}\right), \tag{17}$$

where the PDEM background imposes an additional restriction $a > -1/2$ on the wavefunctions again.

Turning now to the initial potential $V(x)$, we find from Eq. (2) that $V(x) = V_{\rm eff}(x) + q^2[f(\alpha,\beta)\cosh^2 qx - g(\alpha,\beta)]$ and $V(x) = V_{\rm eff}(x) + \frac{1}{4}q^2 f(\alpha,\beta)e^{qx}$, with $f(\alpha,\beta) \equiv (2\alpha+1)(2\alpha+2\beta+2) - 2\alpha$, $g(\alpha,\beta) \equiv (2\alpha+1)^2 + \beta(4\alpha+1)$, for the Jacobi and generalized Laguerre polynomials, respectively. Hence, in both cases, for the choice of ambiguity parameters made by BenDaniel and Duke ($\alpha = 0$, $\beta = -1$) [22], there is no distinction between $V(x)$ and $V_{\rm eff}(x)$. Furthermore, when the Jacobi polynomials reduce to Legendre ones, i.e., for $a = b = 0$, and the ambiguity parameters are those selected by Zhu and Kroemer ($\alpha = -1/2$, $\beta = 0$) [23], $V(x)$ becomes a constant potential V_0. Our results (10) and (12) then describe the generation of an infinite number of bound states for a free-particle potential in a sech^2-mass environment [14]. For nonvanishing a, b values, Eqs. (10)–(12) may therefore be seen as a generalization of this interesting property.

4 Generation of QES potentials in the $M = \lambda/g'$ case

Whenever $M = \lambda/g'$, Eq. (6) becomes

$$E - V_{\rm eff}(x) = \frac{g'''}{\lambda} - \frac{g''^2}{\lambda g'} + \frac{g'^3}{\lambda}\left(R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2\right). \tag{18}$$

In such a case, we shall take for $F(g)$ some polynomials of nonhypergeometric type satisfying the equation

$$\ddot{F} + \frac{a(g^2-\xi^2)}{g^3}\dot{F} + \frac{bg+c}{g^3}F = 0, \tag{19}$$

where we assume a, b, c, ξ real, $a \neq 0$, $b \neq 0$ and $\xi > 0$. As shown elsewhere [24], this second-order differential equation has kth-degree polynomial solutions provided $b = -k(a+k-1)$ and there exist $k+1$ such solutions $F_n(g)$, $n = 0, 1, \ldots, k$, associated with $k+1$ distinct values c_n of c, if a is appropriately chosen.

Substituting

$$R - \frac{1}{2}\dot{Q} - \frac{1}{4}Q^2 = -\frac{(2k+a-2)(2k+a)}{4g^2} + \frac{c_n}{g^3} + \frac{a(a-3)\xi^2}{2g^4} - \frac{a^2\xi^4}{4g^6} \tag{20}$$

in Eq. (18), we find a constant term on the right-hand side of the transformed equation by choosing $g'^3/(\lambda g^3) = C$. Then with $C = q^2$ and $\lambda = q > 0$, we obtain

$$g(x) = e^{qx}, \qquad M(x) = e^{-qx}, \qquad -\infty < x < +\infty. \tag{21}$$

Hence

$$\begin{aligned} E_n &= q^2 c_n + V_0, & (22)\\ V_{\rm eff}(x) &= q^2\left[\frac{1}{4}(2k+a-2)(2k+a)e^{qx} - \frac{1}{2}a(a-3)\xi^2 e^{-qx} + \frac{1}{4}a^2\xi^4 e^{-3qx}\right] + V_0, & (23)\\ \psi_n(x) &\propto \exp\left[\frac{1}{2}(a-2)qx + \frac{1}{4}a\xi^2 e^{-2qx}\right] F_n\left(e^{qx}\right), & (24) \end{aligned}$$

where $n = 0, 1, \ldots, k$.

The functions (24) turn out to be physically acceptable as bound-state wavefunctions provided a is restricted to the range $a < -2k + \frac{3}{2}$. We conclude that for such values and for the PDEM given in (21), the effective potentials (23) corresponding to $k = 1, 2, 3, \ldots$, are QES with $k+1$ known eigenvalues and eigenfunctions. For $k = 1$ and $k = 2$, for instance, we find

$$c_{\substack{0\\1}} = \pm a\xi, \qquad F_{\substack{0\\1}}(g) \propto g \pm \xi, \qquad \text{if } a < -\frac{1}{2}, \tag{25}$$

and

$$\begin{aligned} c_{\substack{0\\2}} &= \mp\Delta\xi, \qquad c_1 = 0, \qquad F_{\substack{0\\2}}(g) \propto g^2 \mp \frac{\Delta}{a+2}\xi g + \frac{a}{a+2}\xi^2, \\ F_1(g) &\propto g^2 - \frac{a}{a+1}\xi^2, \qquad \Delta \equiv \sqrt{2a(2a+3)}, \qquad \text{if } a < -\frac{5}{2}, & (26) \end{aligned}$$

respectively. Observe on these two examples that for the values taken by a, ξ and $g(x)$, $\psi_n(x)$ has n zeros on the real line, so that $\psi_0(x)$ is the ground-state wavefunction, while $\psi_n(x)$, $n = 1, 2, \ldots, k$, correspond to the nth excited states.

The results presented here could be easily extended to more general polynomials. For instance, if instead of $g^2 - \xi^2$ in (19), we had considered $(g - g_3)(g - g_4)$ with g_3 and g_4 real but $g_4 \neq -g_3$, we would have obtained effective potentials containing an additional term proportional to e^{-2qx}.

Finally, it should be noticed that the PDEM being the same as that chosen for generalized Laguerre polynomials in Sec. 3, the relation between $V(x)$ and $V_{\rm eff}(x)$ is also similar.

5 SUSYQM approach

Let us consider the intertwining relationship $\eta H = H_1 \eta$, where H is the Hamiltonian defined in Eq. (1), H_1 has the same kinetic energy term but an associated effective potential $V_{1,\rm eff}(x)$, and η is a first-order intertwining operator $\eta = A(x)\frac{d}{dx} + B(x)$. As shown in [14], such a relationship leads to the restrictions $A(x) = M^{-1/2}$ and

$$V_{\rm eff}(x) = \epsilon + B^2 - \left(\frac{B}{\sqrt{M}}\right)', \qquad V_{1,\rm eff}(x) = V_{\rm eff} + \frac{2B'}{\sqrt{M}} + \frac{M''}{2M^2} - \frac{3M'^2}{4M^3}, \tag{27}$$

with ϵ denoting some arbitrary constant.

A solution for $B(x)$, which at the same time ensures that η annihilates the ground-state wavefunction of H, is provided by $B(x) = -\psi_0'/(\sqrt{M}\psi_0)$ together with $\epsilon = E_0$. In this (PDEM-extended) unbroken SUSYQM framework [25], the eigenvalues of H_1 are $E_{1,n} = E_{n+1}$, $n = 0, 1, 2, \ldots$, with the corresponding wavefunctions given by $\psi_{1,n} \propto \eta\psi_{n+1}$.

For the wavefunctions considered in Eq. (3), ψ_0'/ψ_0 in general contains two terms: $\psi_0'/\psi_0 = f'/f + g'\dot{F}_0/F_0$. In the ES potential case reviewed in Sec. 3, however, the second term vanishes since $F_0(g) = 1$, so that we obtain simple results for $B(x)$, namely

$$B(x) = \frac{1}{2}q[(a-b)\cosh qx + (a+b+2)\sinh qx] \tag{28}$$

and

$$B(x) = \frac{1}{2}q[(a+1)e^{qx/2} - e^{-qx/2}] \tag{29}$$

for the Jacobi and generalized Laguerre polynomials, respectively. Substituting such functions in (27), we arrive at SUSY partners $V_{1,\mathrm{eff}}(x)$, which have the same shape as $V_{\mathrm{eff}}(x)$ and differ only in the parameters ($a_1 = a+1$, $b_1 = b+1$, $V_{0,1} = V_0$ and $a_1 = a+1$, $V_{0,1} = V_0 + \frac{1}{2}q^2$, respectively). We conclude that the potentials $V_{\mathrm{eff}}(x)$ are shape invariant.

The QES potential case reviewed in Sec. 4 looks more interesting because $F_0(g)$ being now a kth-degree polynomial in g, the second term in ψ_0'/ψ_0 does not vanish anymore. As a consequence, the functions $B(x)$ and $V_{1,\mathrm{eff}}(x)$ become k-dependent and given by

$$\begin{aligned} B(x) &= q\left[-\frac{1}{2}(a-2)e^{qx/2} + \frac{1}{2}a\xi^2 e^{-3qx/2} - e^{3qx/2}\frac{\dot{F}_0}{F_0}\right], && (30) \\ V_{1,\mathrm{eff}}(x) &= V_{\mathrm{eff}} - q^2\left[\frac{1}{2}\left(a-\frac{3}{2}\right)e^{qx} + \frac{3}{2}a\xi^2 e^{-qx} + 3e^{2qx}\frac{\dot{F}_0}{F_0} + 2e^{3qx}\left(\frac{\ddot{F}_0}{F_0} - \frac{\dot{F}_0^2}{F_0^2}\right)\right]. && (31) \end{aligned}$$

The SUSY partners $V_{1,\mathrm{eff}}(x)$ therefore contain some terms which are rational functions in e^{qx}. For $k=1$ and $k=2$, for instance, we obtain

$$\begin{aligned} V_{1,\mathrm{eff}}(x) &= q^2\left[\frac{1}{4}(a-1)(a+1)e^{qx} - \frac{1}{2}a^2\xi^2 e^{-qx} + \frac{1}{4}a^2\xi^4 e^{-3qx} \right. \\ &\quad \left. + \frac{3\xi^2}{e^{qx}+\xi} - \frac{2\xi^3}{(e^{qx}+\xi)^2}\right] + V_0 - q^2\xi \qquad (32) \end{aligned}$$

and

$$\begin{aligned} V_{1,\mathrm{eff}}(x) &= q^2\left[\frac{1}{4}(a+1)(a+3)e^{qx} - \frac{1}{2}a^2\xi^2 e^{-qx} + \frac{1}{4}a^2\xi^4 e^{-3qx} \right. \\ &\quad \left. + \frac{a\xi^2}{(a+2)^3}Z_1(x) - \frac{4a^2\xi^4}{(a+2)^4}Z_2(x)\right] + V_0 + q^2\frac{\Delta\xi}{a+2}, \\ Z_1(x) &\equiv \frac{6(a+2)(a+1)e^{qx} - (a+6)\Delta\xi}{e^{2qx} - \frac{\Delta}{a+2}\xi e^{qx} + \frac{a}{a+2}\xi^2}, \\ Z_2(x) &\equiv \frac{(3a+4)e^{qx} - \Delta\xi}{\left(e^{2qx} - \frac{\Delta}{a+2}\xi e^{qx} + \frac{a}{a+2}\xi^2\right)^2}, \qquad (33) \end{aligned}$$

respectively. Such effective potentials provide us with some new examples of QES potentials in a PDEM environment with k known eigenvalues and eigenfunctions.

6 Conclusion

In this Letter, we have investigated the problem of the one-dimensional Schrödinger equation in a PDEM background from several viewpoints. By using first the PCT approach and

assuming a relation between the new variable $g = g(x)$ and the mass $M(x)$ that differs from the usual one, we have constructed some new ES or QES potentials. The former are associated with either Jacobi or generalized Laguerre polynomials, while the latter correspond to some kth-degree polynomials of nonhypergeometric type.

We have then considered an equivalent intertwining-operator approach and shown that while our ES potentials are shape invariant, the SUSY partners of our QES potentials are new. In the latter case, iterating the procedure would lead us to a hierarchy of SUSY partners with an increasingly complicated form.

The method described here could be used to generate other classes of masses and potentials providing exact solutions of the PDEM Schrödinger equation.

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